

L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN  
RN 31906-04-4 REGISTRY  
ED Entered STN: 16 Nov 1984  
CN 3-Cyclohexene-1-carboxaldehyde, 4-(4-hydroxy-4-methylpentyl)- (CA INDEX NAME)

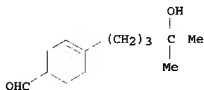
OTHER NAMES:

CN 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexene-1-carboxaldehyde  
CN 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexenecarboxaldehyde  
CN 4-(4-Methyl-4-hydroxyamyl)cyclohex-3-ene carboxaldehyde  
CN Liral  
DR 56493-02-8, 80449-98-5  
MF C13 H22 O2  
LC STN Files: ANABSTR, BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM, CSNB, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, PROMT, RTECS\*, SCISEARCH, TOXCENTER, USPAT2, USPATFULL, USPATOLD

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

171 REFERENCES IN FILE CA (1907 TO DATE)  
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
172 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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DT.CA Caplus document type: Conference; Journal; Patent

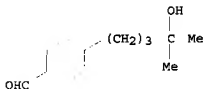
RL.P Roles from patents: BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	
C6	C6	6	C6	46.150.2	1



Experimental Properties (RPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Boiling Point (BP)	120 deg C	Press: 1 Torr	(1) CAS
Density (DEN)	0.9941 g/cm**3		(1) CAS
Refractive Index (RI)	1.4915	Temp: 20 deg C	(1) CAS
		Wavlen: 589.3 nm	

(1) Teegarden, Robert W.; US 2947780 1960 CAPLUS

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
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Bioconc. Factor (BCF)	49.44	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	49.44	pH 10 25 deg C	(1)
Boiling Point (BP)	318.7+/-42.0 deg C	760 Torr	(1)
Density (DEN)	1.023+/-0.06 g/cm**3	20 deg C	(1)
		760 Torr	
Enthalpy of Vap. (HVAP)	64.94+/-6.0 kJ/mol		(1)
Flash Point (FP)	135.1+/-20.5 deg C		(1)
Freely Rotatable Bonds (FRB)	6		(1)
H acceptors (HAC)	2		(1)
H donors (HD)	1		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	3		(1)
Koc (KOC)	567.49	pH 1 25 deg C	(1)
Koc (KOC)	567.49	pH 2 25 deg C	(1)
Koc (KOC)	567.49	pH 3 25 deg C	(1)
Koc (KOC)	567.49	pH 4 25 deg C	(1)
Koc (KOC)	567.49	pH 5 25 deg C	(1)
Koc (KOC)	567.49	pH 6 25 deg C	(1)
Koc (KOC)	567.49	pH 7 25 deg C	(1)
Koc (KOC)	567.49	pH 8 25 deg C	(1)
Koc (KOC)	567.49	pH 9 25 deg C	(1)
Koc (KOC)	567.49	pH 10 25 deg C	(1)
LOGD (LOGD)	2.53	pH 1 25 deg C	(1)
LOGD (LOGD)	2.53	pH 2 25 deg C	(1)
LOGD (LOGD)	2.53	pH 3 25 deg C	(1)
LOGD (LOGD)	2.53	pH 4 25 deg C	(1)
LOGD (LOGD)	2.53	pH 5 25 deg C	(1)
LOGD (LOGD)	2.53	pH 6 25 deg C	(1)
LOGD (LOGD)	2.53	pH 7 25 deg C	(1)
LOGD (LOGD)	2.53	pH 8 25 deg C	(1)
LOGD (LOGD)	2.53	pH 9 25 deg C	(1)
LOGD (LOGD)	2.53	pH 10 25 deg C	(1)
LOGP (LOGP)	2.532+/-0.257	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.63 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.63 g/L	Unbuffered Water	(1)
		pH 7.00	
		25 deg C	
Molar Intrinsic Solubility (ISLB.MOL)	0.0030 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 5 25 deg C	(1)

Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0030 mol/L	Unbuffered Water	(1)
		pH 7.00	
Molar Volume (MVOL)	205.4+/-3.0 cm**3/mol	25 deg C	(1)
		20 deg C	
		760 Torr	
Molecular Weight (MW)	210.31		(1)
PKA (PKA)	15.31+/-0.29	Most Acidic	(1)
		25 deg C	
Polar Surface Area (PSA)	37.30 A**2		(1)
Vapor Pressure (VP)	2.94E-05 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14  
{(C) 1994-2008 ACD/Labs}

See HELP PROPERTIES for information about property data sources in REGISTRY.

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